Interatomic distances, atoms involves, bond critical points for all the complexes $S(CH_3)_2$:YOH (Y=F, Cl, Br, I) obtained with AIM theory at MP2/aug'-cc-pVTZ level of theory.

YOH	Conf.	Dist.	Atoms	r	Lap
F	I	-	-	-	-
Cl	I	2.170	H-S	0.033	0.046
Br	I	2.129	H-S	0.036	0.047
I	I	2.173	H-S	0.033	0.047
F	II	2.206	H-S	0.031	0.046
		2.632	H-F	0.006	0.023
		2.632	H-F	0.006	0.023
Cl	II	2.199	H-S	0.032	0.045
		3.039	H-Cl	0.005	0.019
		3.039	H-Cl	0.005	0.019
Br	II	2.175	H-S	0.033	0.046
		3.060	H-Br	0.007	0.021
		3.060	H-Br	0.007	0.021
I	II	2.225	H-S	0.030	0.046
		3.312	H-I	0.006	0.016
		3.312	H-I	0.006	0.016
F	III				
Cl	III	2.598	H-O	0.006	0.025
		2.598	H-O	0.006	0.025
Br	III	2.471	H-O	0.008	0.031
		2.471	H-O	0.008	0.033
I	III				
F	IV_a	3.212	F-S	0.007	0.028
		2.621	H-F	0.006	0.024
		2.621	H-F	0.006	0.024
F	IV_b	3.555	F-S	0.004	0.016
		2.618	H-F	0.006	0.022
		2.618	H-F	0.006	0.022
Cl	IV	2.798	Cl-S	0.033	0.075
Br	IV	2.684	Br-S	0.048	0.078
I	IV	2.854	I-S	0.042	0.065
F	V	-	-	-	-
Cl	V	-	-	-	-
Br	V	-	-	-	-

I	V	2.854	I-S	0.042	0.065

Interatomic distances, atoms involves, bond critical points for all the complexes $Se(CH_3)_2$:YOH (Y=F, Cl, Br, I) obtained with AIM theory at MP2/aug'-cc-pVTZ level of theory.

	Conf.	Dist.	Atoms	r	Lap
F	I	-	-	-	-
Cl	I	3.147	H - Cl	0.005	0.019
		2.266	H - Se	0.032	0.040
Br	I	2.196	H - Se	0.036	0.040
I	I	2.265	H - Se	0.032	0.041
F	II	2.308	H - Se	0.029	0.039
		2.609	H - F	0.006	0.023
		2.609	H - F	0.006	0.023
Cl	II	2.297	H - Se	0.030	0.039
		3.017	H - Cl	0.006	0.019
		3.017	H - Cl	0.006	0.019
Br	II	2.253	H - Se	0.033	0.040
		3.028	H - Br	0.007	0.022
		3.028	H - Br	0.007	0.022
I	II	2.318	H - Se	0.029	0.040
		3.293	H - I	0.006	0.016
		3.293	H - I	0.006	0.016
F	III	-	-	-	-
Cl	III	2.547	H - O	0.007	0.028
		2.547	H - O	0.007	0.028
Br	III	2.439	H - O	0.009	0.036
		2.439	H - O	0.009	0.036
I	III	-	-	-	-
F	IV	3.235	F - Se	0.008	0.030
		2.605	H - F	0.006	0.025
		2.605	H - F	0.006	0.025
Cl	IV	2.819	Cl - Se	0.036	0.069
Br	IV	2.726	Br - Se	0.050	0.067
I	IV	2.928	I - Se	0.041	0.055
F	V	-	-	-	-
Cl	V	-	-	-	-
Br	V	-	-	-	-
I	V	2.927	I - Se	0.042	0.055

Interatomic distances, atoms involves, bond critical points for all the complexes $Te(CH_3)_2$:YOH (Y=F, Cl, Br, I) obtained with AIM theory at MP2/aug'-cc-pVTZ/aug-cc-pVTZ-PP level of theory.

	Conf.	Dist.	Atoms	r	Lap
F	I	-	-	-	-
Cl	I	2.484	H-Te	0.026	0.032
Br	I	2.479	H-Te	0.027	0.032
I	I	2.498	H-Te	0.026	0.032
F	II	2.533	H-Te	0.024	0.031
		2.632	H-F	0.006	0.022
		2.632	H-F	0.006	0.022
Cl	II	2.511	H-Te	0.025	0.031
		3.027	H-Cl	0.006	0.018
		3.027	H-Cl	0.006	0.018
Br	II	2.512	H-Te	0.025	0.031
		3.124	H-Br	0.006	0.018
		3.124	H-Br	0.006	0.018
I	II	2.540	H-Te	0.024	0.032
		3.295	H-I	0.006	0.016
		3.295	H-I	0.006	0.016
F	III	-	-	-	.
Cl	III	2.490	H-O	0.008	0.032
		2.490	H-O	0.008	0.032
Br	III	2.448	H-O	0.009	0.036
		2.448	H-O	0.009	0.036
I	III	-	-	-	-
F	IV	3.363	F-Te	0.008	0.026
		2.593	H-F	0.006	0.025
		2.593	H-F	0.006	0.025
Cl	IV	2.830	Cl-Te	0.044	0.056
Br	IV	2.873	Br-Te	0.047	0.049
I	IV	3.060	I-Te	0.040	0.042
F	V	-	-	-	-
Cl	V	-	-	-	-
Br	V	-	-	-	-
I	V	3.059	I-Te	0.041	0.042

SAPT-DFT energy decomposition for all the complexes $S(CH_3)_2$:YOH (Y=F, Cl, Br, I) at MP2/aug'-cc-pVTZ/aug-cc-pVTZ-PP level of theory.

	Conf.	$E_{el}^{(1)}$	$E_{ex}^{(1)}$	$E_i^{(2)}$	$E_D^{(2)}$	δ(HF)	$\Delta E^{DFT-SAPT}$
F	I						
Cl	I	-47.94	65.98	-14.13	-25.03	-11.55	-32.66
Br	I	-51.96	77.58	-15.48	-29.14	-12.47	-31.46
I	I	-48.12	69.35	-15.10	-27.84	-8.77	-30.48
F	II	-48.54	61.24	-13.76	-22.09	-11.41	-34.56
Cl	II	-50.05	66.61	-13.83	-25.75	-11.55	-34.56
Br	II	-54.41	77.70	-14.61	-29.59	-12.34	-33.25
I	II	-49.48	68.70	-14.41	-27.99	-8.22	-31.39
F	III	-4.69	10.40	-0.47	-9.35	-0.63	-4.75
Cl	III	-8.29	15.54	-0.50	-13.15	-0.98	-7.37
Br	III	-12.38	25.61	-0.78	-17.93	-1.58	-7.05
I	III						
F	IV	-6.34	13.16	-0.30	-9.53	-1.55	-4.56
Cl	IV	-65.41	115.65	-11.85	-32.27	-22.50	-16.38
Br	IV	-132.45	222.20	-54.47	-47.11	-16.96	-28.79
I	IV	-133.00	164.68	-184.02	-45.16	152.08	-45.42
F	V						
Cl	V						
Br	V						
I	V	-132.56	164.77	-184.54	-45.01	152.97	-44.37

SAPT-DFT energy decomposition for all the complexes $Se(CH_3)_2$:YOH (Y=F, Cl, Br, I) at MP2/aug'-cc-pVTZ/aug-cc-pVTZ-PP level of theory

	Conf.	$E_{el}^{(1)}$	$E_{ex}^{(1)}$	$E_i^{(2)}$	$E_D^{(2)}$	δ(HF)	$\Delta E^{DFT-SAPT}$
F	I						
Cl	I	-47.62	68.41	-14.36	-25.77	-11.80	-31.14
Br	I	-53.85	86.30	-16.95	-31.49	-13.26	-29.26
I	I	-48.60	72.65	-16.64	-29.51	-7.62	-29.72
F	II	-47.76	62.90	-13.82	-22.53	-11.73	-32.94
Cl	II	-50.04	69.53	-14.04	-26.59	-11.94	-33.08
Br	II	-56.95	85.97	-15.69	-31.54	-13.27	-31.48
I	II	-50.65	72.82	-16.06	-29.97	-7.32	-31.19
F	III						
Cl	III	-8.97	17.40	-0.58	-14.29	-1.10	-7.55
Br	III	-13.66	29.11	-0.91	-19.67	-1.79	-6.92
I	III						
F	IV	-7.77	16.74	-0.23	-10.68	-2.36	-4.30

Cl	IV	-82.51	148.47	-18.64	-36.66	-27.47	-16.81
Br	IV	-157.31	265.28	-79.33	-51.52	-6.87	-29.76
I	IV	-146.48	178.74	-231.72	-48.50	203.01	-44.95
F	V						
Cl	V						
Br	V						
I	V	-146.50	179.29	-233.21	-48.39	204.96	-43.84

SAPT-DFT energy decomposition for all the complexes $Te(CH_3)_2$:YOH (Y=F, Cl, Br, I) at MP2/aug'-cc-pVTZ/aug-cc-pVTZ-PP level of theory

	Conf.	$E_{el}^{(1)}$	$E_{ex}^{(1)}$	$E_i^{(2)}$	$E_D^{(2)}$	δ(HF)	$\Delta E^{DFT-SAPT}$
F	I						
Cl	I	-43.65	61.88	-14.05	-24.84	-8.77	-29.42
Br	I	-48.34	72.00	-15.39	-28.96	-7.83	-28.51
I	I	-47.16	67.23	-21.67	-29.27	2.50	-28.38
F	II	-42.09	55.55	-12.82	-21.41	-9.24	-30.02
Cl	II	-47.16	66.38	-13.96	-27.03	-9.36	-31.14
Br	II	-49.99	72.73	-14.61	-29.85	-8.84	-30.55
I	II	-48.25	67.94	-19.73	-30.30	-0.02	-30.36
F	III						
Cl	III	-10.83	22.91	-0.72	-17.45	-1.33	-7.42
Br	III	-13.70	29.73	-0.98	-20.86	-1.71	-7.52
I	III						
F	IV	-9.35	19.63	-0.10	-11.63	-2.87	-4.31
Cl	IV	-122.79	219.46	-49.45	-45.54	-20.39	-18.71
Br	IV	-171.94	279.80	-116.06	-52.90	25.85	-35.25
I	IV	-161.28	184.17	-315.47	-50.55	301.19	-41.94
F	V						
Cl	V						
Br	V						
I	V	-161.96	185.25	-319.17	-50.52	305.15	-41.25